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PHYSICAL CHARACTERIZATION OF ELECTRONIC MATERIALS.(U)
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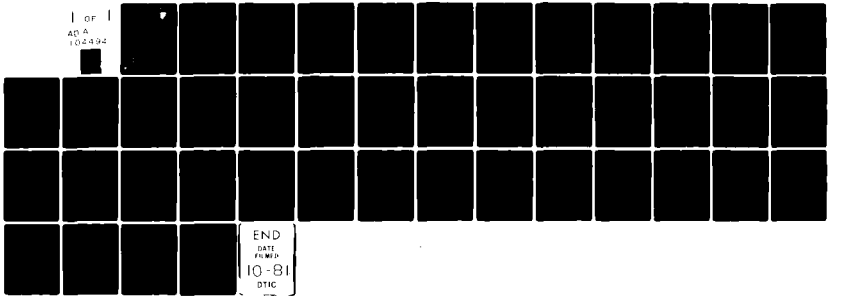

LEVEL II

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RADC-TR-81-167
Final Technical Report
July 1981

PHYSICAL CHARACTERIZATION OF ELECTRONIC MATERIALS

MANLABS, Inc.

S. Andrew Kulin
E.P. Warekois

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER RADC-TR-81-167	2. GOVT ACCESSION NO. AD-A104 494	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) PHYSICAL CHARACTERIZATION OF ELECTRONIC MATERIALS		5. TYPE OF REPORT & PERIOD COVERED Final Technical Report 3 Jan 78 — 30 Sep 80
		6. PERFORMING ORG. REPORT NUMBER N/A
7. AUTHOR(s) S. Andrew Kulin E.P. Warekois		8. CONTRACT OR GRANT NUMBER(s) F19628-78-C-0060
9. PERFORMING ORGANIZATION NAME AND ADDRESS MANLABS, Inc. 21 Erie Street Cambridge MA 02139		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2306J129
11. CONTROLLING OFFICE NAME AND ADDRESS Deputy for Electronic Technology (RADC/ESM) Hanscom AFB MA 01731		12. REPORT DATE July 1981
		13. NUMBER OF PAGES
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) Same		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE N/A

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

Same

18. SUPPLEMENTARY NOTES

RADC Project Engineer: Norman E. Pickering (ESM)

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

electromagnetic	skull melting	thermodynamic
electrooptical materials	semi-conductor alloys	
glass preforms	vapor-liquid-solid	
fiber optics	equilibria	
hydrothermal	cadmium-tellurium mercury system	

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The objectives of the present contract have been to develop or adapt fabrication and measurement techniques for the evaluation of the properties of new electromagnetic or electrooptical materials including new compounds and alloys. This effort has been performed in support of the research programs conducted within the Materials Characterization Branch of the Solid State Sciences Laboratory of the Deputy for Electronic Technology of the Rome Air Development Center.

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The effort expended during this contract can be divided into three main programs. Methods have been developed to fabricate samples from the glass preforms used as source materials for fiber optics and then some analytical methods have been adapted to determine the chemistry of those source materials. Considerable effort was devoted to the fabrication of oriented specimens of seeds, resonators and cells needed for the growth and characterization of hydrothermally grown quartz and some other quartz-like crystals. Several analytical methods have been used in order to obtain data on the characteristics of material grown in a "Skull-melt" type facility. Some work was devoted to the evaluation of new semi-conductor materials and devices. The major effort in those cases involved Auger analysis of deposited films of semi-conductor alloys.

The more general features of the types of experimental methods employed to obtain these data are detailed in several reports referenced in the text of this report. The specific adaptations of features of those methods are discussed under portions of the report.

The requests for such services were individually submitted and the data obtained from such programs was reported to the originator as short letter reports and quarterly summary reports. The context of those reports are included in this final report as a Table of Services. In addition, to the service requests, a lengthy calculation of the vapor-liquid-solid equilibria in the cadmium-tellurium mercury system was performed.

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I. SUMMARY

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II. INTRODUCTION

ManLabs, Inc. has conducted a research program in support of the programs in progress within the Materials Characterization Branch of the Solid State Laboratory of the Deputy for Electronic Technology of the Rome Air Development Center. The work statement for the program indicated that the purpose of the effort was to develop new or adapt existing methods for the fabrication and testing of new electromagnetic materials and alloys. The specific objectives were to develop those methods that would permit the characterization of the chemical, physical and structural properties of the materials being developed or utilized by the programs within the Branch.

The various experimental methods employed in this program have been detailed in previous reports entitled "Physical Characterization of Electron Materials, Devices and Thin Films"-Final Report for contract F19-628-70C-0173 dated November 30, 1969. Several modifications to the basic techniques have been detailed in other reports entitled "Physical Characterization of Electronic Materials"-Final Report for contracts F19-628-70C-0140 and F19-628-77C-0040 dated December 1, 1972 and September 30, 1977.

The present contract was a continuation of the same type of program and was implemented by individual service requests from various staff members for various types of experimental measurements or tasks. All requests could be broadly classed into either a sample preparation task or a chemical analysis request. The list of the services performed during the course of this contract have been listed in Table I. One column of that table does identify the services rendered in terms of one or the other of broad classes of requests.

The scope of the materials investigated during this contract was, of course, defined by the programs in progress under various staff personnel in the Branch or by exploratory work performed in order to define directions or programs for future investigations.

The major classes of materials studied were:

a) Quartz and other crystalline materials that could be grown by hydrothermal methods. The objective of these measurements was to define experimental parameters that would relate the properties to growth parameters or suggest methods that might optimize the parameters of the crystals produced.

b) Feed stock for optical fibers or fiber optic cables was the subject of one major program underway during this contract period. Considerable effort was devoted to the perfection of preparation methods that would permit the inspection of highly strained glass preforms used as the starting material for the drawn fiber. Most of the material used for such fibers are various systems of glass formers so that some chemical analysis programs were initiated in order to monitor the purity or composition of such glasses. Several extensive SEM inspections of the very fine fibers were conducted in order to obtain information on the surface features of the fibers or coatings on the fibers. Similar inspections had been made in order to relate the variations in the chemical composition of the fibers to the optical variations in those same materials.

c) Refractory type materials produced in a "Skull-melt" type facility were considered during this contract. Most of the effort was directed towards the perfection of growth parameters so that pure or doped samples of the yttria stabilized cubic zirconium dioxide could be obtained in reasonable sized lots. Several extensive programs were devoted to the evaluation of optical, chemical and crystalline perfection parameters of such classes of material. The operating features of such a growth process were monitored using the chemical purity of the starting materials or the crystalline materials produced as a guide.

d) Semi-conductor compounds and alloys being produced for use as devices or components were evaluated. The major effort in this class of material was the preparation of seed plates and wafers for the growth and electrical measurement of of single crystal indium phosphide. Special oriented seed geometry was developed in order to define certain growth features of this type of material. Methods were developed for the safe handling of this relatively toxic type of material. An extensive Auger type analysis was conducted in order to obtain data on the surface properties of this phosphide when subjected to various oxidizing medium.

Several SEM and Auger analyses have been made on thin films of germanium-silicon alloys and metal coated silicon devices in order to obtain data on the chemical reactions that could occur during the formation of such surfaces or devices.

e) Windows, jigs and fixtures

Many of the experimental facilities needed for such measurements do involved special instrumentation or processes. Thus several requests involve the preparation of IR transmitting salt windows for Dewars, Cells or electrical measuring systems. Several special spooling systems were devised to handle fibers being pulled in the RADC fiber optic furnaces. Several precise, complex mechanical systems have been provided for the electron beam blanking attachments to an electron microscope, the measurement of losses in acoustical oscillators and fixtures for the manipulation of stock into the Skull furnaces. The service requests under this classification have ranged from glasses through soft, salt materials to refractory metals and alloys. The necessary engineering design work was performed as required in order to produce the requested component or system.

f) Thermodynamic Calculations

A thermodynamic calculation of the vapor, liquid, and solid phases of zinc blende structures in the cadmium-mercury-telluride

system was performed. The calculations and data are enclosed as an Appendix to this report.

III. EXPERIMENTAL METHODS

a) Fabrication Techniques

In order to meet the great variety of requests for the processing of a wide range of materials, ManLabs, Inc. has accumulated and developed a number of different types of systems for cutting, polishing or grinding materials. The machines range from wet-string saws for the sectioning of water-soluble materials to multi-wire free abrasive saws for cutting either extremely brittle or hard materials. These cutting saws can be used with almost any type cut-off wheel and during the course of the present contract, steel slitting saws, silicon carbide, diamond and borazon wheels have been employed.

Similarly, ManLabs has a wide range of polishing, grinding or buffing facilities to further process such materials. These systems range from conventional metallurgical polishing wheels to commercially available free-abrasive bowl polishers which include work laps for both plane and curved surfaces.

In most cases, the ultimate surfaces are required to be finished to optical tolerances. For those requests, a multi-spindle Strasbaugh Optical polisher has been used.

A wide variety of jigs and fixtures have been developed for the processing of non-planar shapes and specimens. Some of the optical surfaces and geometries that have been developed for the acoustical devices requirements are unique geometries.

The selection of suitable abrasives, polishing compounds and chemical etches has been made and developed during the processing. In many cases, it was necessary to develop methods for the processing of complex or very small specimens. The processing of fiber optic preforms which are

very highly strained multi-layer depositions of materials inside of a glass tube, required the development of methods to section the tubes without having the hoop-stresses in the sample shatter the samples. Several methods have been developed for the mounting and cross-sectioning of 30 micron diameter fibers taken from optical cables.

The fact that many of the materials processed were toxic cannot be overemphasized. Special venting and washing systems were developed for the cutting and processing of indium phosphide and gallium arsenide crystals. It is extremely important that proper instructions be made available before such materials are handled. A wide and diversified background in materials is available among the ManLabs staff for the dissemination of such information.

b) X-ray Diffraction Methods

The identification of crystallographic phases or the measurements of lattice parameters have been carried out using most of the standard X-ray diffraction methods in use today. Small quantities of materials were examined using Debye-Scherrer film type analysis while larger amounts of material were measured on wide-angle X-ray diffractometers. In either case, the experimentally determined "d" values could be used to identify the crystallographic structures present in the materials.

The crystallographic orientation of surfaces were performed using either the standard back reflection Laue techniques or spectrometer measurements. Since the first method is based on measurements on films the accuracy is limited to about (+/-)1/2°. For those applications that required more accurate definition of surfaces or required known directions within the crystallographic plane, X-ray diffractometer measurements were used. Techniques have been developed that utilize a horizontal diffractometer system in which the θ and 2θ motions are independent of each other. Bond barrel holders, a specialized type of orientation fixture,

have been adapted to such a system and it is now possible to define crystallographic surfaces so that they correspond to the physical surfaces within 10 minutes of arc.

Fixtures have been adapted to the various X-ray diffraction systems so that the long seed rods needed for the InP growth programs plus the various surfaces of quartz transducers could be accurately defined by X-ray measurements.

c) Electron Probe Microanalysis

The electron probe microanalyzer is utilized to determine the chemical composition of a specimen volume about one micron in diameter. In principle, a finely focussed electron beam impinges on the specimen (evacuated chamber) and converts its energy to x-rays which are characteristic of the specimen elements. These x-rays are dispersively analyzed by means of analyzing crystals to yield identification of the x-rays and thus, the specimen elements.

The instrument at ManLabs is capable of analyzing for all elements from boron (Z=5) to uranium (Z=92). Analyses can be qualitative or quantitative. The method is nondestructive and can be used for chemical identification and for chemical distributions as a function of distance.

d) Scanning Electron Microscopy and Energy Dispersive Analysis

A large number of the investigations required the use of a scanning electron microscope in order to obtain high resolution detailed photographs of features or characteristics of the materials. An AMRAY Model 1000A Scanner which incorporated back scatter, secondary electrons and x-ray emission detectors was used for such investigations. The microscope also permitted dual screen, dual magnification photographs to be obtained and incorporated features that permitted the optimization of photographs using gamma intensity control and tilt correction features. Photographs could be routinely obtained at magnifications in the range of 1500

to 2000, while the ultimate magnification ranges were in the 20000 to 30000 range under good experimental conditions.

This particluar SEM system was augmented with an energy dispersive detector and associated microprocessing capabilities. The X-ray spectrum generated when the sample was irradiated with the electron beam could be viewed in real time or stored on magnetic storage disks.

The X-ray data which gives the chemical composition of the area of interest could be accumulated from any position on the sample and that position related to some physical feature on the sample, i.e. a grain boundary, a second phase material or an inclusion or flaw in the material. Once the data had been accumulated the features within the software of the microprocessor would permit one to identify the chemical elements present and using appropriate analytical procedures, the amounts of those elements in terms of weight percent or other quantitative descriptions of the composition.

The particular analytical programs available for such analyses can be used with standards generated by experimentally collecting data from known standard samples, can be used to obtain ratios between samples of known or unknown compositions and can be used to obtain chemical composition based on calculated values based on the operating parameters of the instrument and independent of any experimental or standard X-ray data. The literature has shown that the latter type of analysis - NOST (No standards) is in most cases as significant as data obtained from empirically collected standard data.

e) Other Chemical Analysis Systems

In many cases, the bulk or average chemical composition of materials have been required and at sensitivity levels beyond those possible in the X-ray diffraction scanning microscope/EDAX types of analysis. In those cases, compositional data have been obtained using any variety of optical spectroscopy methods, atomic absorption methods or combustion type analytical procedures. Spectrographic data have been

obtained on Jarrell-Ash Optical Emission units equipped with either spark, arc, graphite furnace or inductively coupled argon plasma sources. These types of procedures do permit measurements in the low ppm range. In some specialized measurements a Perkin-Elmer Model 305 B Atomic Absorption Spectrophotometer has been used. In the case of either gas analysis or carbon analysis in solids, the various types of Leco combustions systems have been used. Data can be obtained from the Leco Model CS-44 (Carbon or Sulfur), the Model TC (Oxygen or Nitrogen) or the Model RH2 (Hydrogen).

f) Auger Analysis

Data has been obtained for the analysis of the surface layers on oxidized semi-conductors and the diffusion profile on platinum-silcide barriers in other semi-conductor devices. The data has been obtained on a PHI type Auger spectrometer capable of sputter etching to controlled depths and the continuous monitoring of up to five species of Auger electrons being ejected from the surfaces. The data obtained from such analysis have been submitted as two reports noted in Table I.

IV. EXPERIMENTAL RESULTS

All data generated during the characterization of any material or device was incorporated into the letter report of that investigation and that report was then distributed to the originator of the request. A total of 201 service requests were processed during the course of this contract. The reports ranged from simple experimental measurements of a data point to extensive in-depth programs covering many facets of a characterization program. The nature of the requests are noted in Table I and the findings summarized below:

a) Materials Produced in the RADC Hydrothermal Growth Systems

Several crystallites of aluminum phosphate, an analog of quartz, were characterized as to their growth

features and oriented plates were obtained from such materials. Those plates were ultimately used in RADC programs that were involved with the development of piezoelectric oscillators that would have zero temperature shifts in the frequency output of the oscillators. It was found that orientation geometries calculated using the piezoelectric coefficient of the materials could be experimentally defined and the operating parameters of those devices were in fair agreement with calculated values.

Extensive sectioning of quartz boules grown under different conditions was performed on RADC grown materials in order to evaluate growth parameters and the distribution of impurities in such grown materials. Material obtained from other sources, supplied to us by RADC, did show that it was possible to prepare seed plates by optical polishing such that the new growth/seed plate interfaces could not be seen under normal inspection conditions. Most of the quartz plates processed under this contract have been subjected to measurements at the RADC facilities with very little of that type of experimental data being generated at ManLabs, Inc.

b) Analysis of Fiber Optic Cables and Materials

The stock material for fiber optic cables usually consists of layers of various materials which have been CVD deposited on silia tubes and the tubes are then drawn down to produce solid cores of interleaved layers of material designed to give the cable the required optic variation. This structure called a "preform" is a highly stressed series of concentric surfaces and is difficult to section for any kind of examination. However, during this contract,methods have been developed using extremely slow feed speeds on diamond wheels so that sections could be prepared for future internal examinations. Electron beam microprobe traces and SEM examinations of such cross-sections have shown that the observed optical variations across the preform correspond to

compositional variations. An extensive examination of several different compositions of glass preforms was presented as reports for service request #04556,#04570, #04577 and #04578. Several techniques have been developed in order to mount, polish and examine the cross-section of individual fibers using either optical or SEM instruments for such examinations. Several requests involved the careful examination of fiber optic cables coated with a very hard carbon-like material.

The later phase of the contract involved considerable analytical effort in order to determine the chemical impurity levels in the ppm range in starting powders used to prepare the glass sources for the fibers. It was determined that inductively coupled plasma emission sources could provide such types of analyses. However, one serious limitation in such analysis was the methods used to completely digest the glass samples so that the solutions could be fed through the plasma torch. Several lots of materials have been analyzed and the data was found to be in good agreement with data provided by extensive measurements on similar standards by the National Bureau of Standards. It was found that SEM/EDAX analysis could be used for semi-quantitative data relative to the multi-component fluoride glass sources used as IR transmitting glasses.

c) Materials Produced in the RADC "Skull-Melt" Facilities

Extensive investigations have been performed on various lots of yttria stabilized zirconium dioxide crystals grown by the Skull-melt procedure. (Request 04547) Data obtained on the optical properties, the density, the X-ray parameters and the thermal properties of material produced indicated that at least 10-11 weight percent of yttria was needed to stabilize the cubic phase and produce solid, sound sections of crystallized material. Any additions over that minimum value did not seem to significantly change any of the properties of the crystalline material.

Measurements of the optical constants of the material were made using ellipsometry methods and the data so obtained agreed with published values for the index of refraction measured by more conventional methods. Thermal conductivity data was obtained using a relatively new contact type measurement in which the conductivity is determined from the heat flow needed to maintain a constant temperature in a thermistor contacting the surface. The measured heat flow is then compared to calibration materials with known thermal conductivity values. The data obtained on both doped and zirconium dioxide crystals are in the range of 0.017-0.019 watts/cm/°C.

It was found that several lots of solidified zirconium dioxide crystalline material contained regions with a very different type of crystal morphology. Such features were especially noted in those samples doped with various amounts of rare earths. The chemical analyses of such crystals were not conclusive enough to show the effect was due to impurity segregation at the grain boundaries. Since the regions were characterized by very fine grain structures, it is suggested that thermal variations across the surface of the solidifying melt are a more likely cause of these areas.

One inherent advantage of the Skull method is the absence of a crucible or container hence there is less chance of impurity pick-up from the walls of such containers. Several attempts have been evaluated in an attempt to melt silicon in the Skull configuration and to then extend the method to the production of silicon-germanium alloys. The initial results have indicated that the method can be used to melt and even alloy the components, but the differences in thermal expansion between the silicon and germanium caused the silicon being used as the crucible to crack. An examination did show there was a reaction and alloy compositions from 15 to 20 weight percent of silicon in germanium had been produced.

d) Auger Analysis

The chemical composition of surfaces as a function of depth have been determined for several types of diffusion control processes involved in the fabrication or treatment of semi-conductor devices. The method is based on the monitoring of the Auger electrons emitted as the surfaces are subjected to Argon ion bombardment. The method is capable of monitoring up to seven species of elements as a function of sputtering time which after calibration is a direct measure of the thickness of surface being removed.

In one program it was found that phosphorous in a base InP substrate would diffuse through oxidized layers produced on the InP even up to thicknesses about 1000 to 14000 Å of the oxide. Thus the electrical properties of the normally non-conductive surfaces can be greatly altered by such diffusion profiles.

A similar investigation has shown that the diffusion of platinum into silicon wafers proceeds by the formation of a silicide. The diffusion zones can be factors of two greater than the original thickness of metal deposited on the silicon surface.

Details of these two studies have been incorporated into reports issued in conjunction with requests #04674 and #04708.

e) Semi-Conductor Materials

The investigations in this area have been restricted to the indium phosphide materials in order to support those crystal growing facilities at RADC. One aspect of the program was the fabrication of seed rods with orientations off the major poles in an attempt to produce crystals that would have the inherent twin plane orientation. Several (115) seed rods have been produced for such growths.

An extensive program reported as part of request #04636,#04650,#04652 involved the SEM/EDAX characterizations

of both the morphology and chemical compositions of about 75 silicon wafers onto which had been deposited germanium. The depositions were then subsequently treated in order to produce variations in the surface features and chemical composition of the silicon-germanium alloys formed. Methods were developed using EDAX type analysis that did show some correlations between the chemical composition and the types of surfaces formed.

f) Thermodynamic Calculations

Attached is a self-contained report relative to the calculation of vapor-liquid phase equilibria in the system containing cadmium-mercury-and tellerium as a function of both temperature and pressure.

TABLE I

List of Services and Materials

Item 1 - Item 201

January 3, 1978 through September 30, 1980

Item	RADC No.	Requestor	Material	Specimen	Type of Service
1	04517	A. Armington	Quartz	AJ	Opt. Fab.
2	04518	H. Lipson	MgF_2	OPTO#8	Opt. Fab.
3	04519	H. Lipson	Quartz	2C/3C	Opt. Fab.
4	04520	R. Hilton	InP	12:13:77	X-Ray:Fab.
5	04521	H. Lipson	NaCl	(2)	Opt. Fab.
6	04522	H. Lipson	MgF_2	OPTO#8	Opt. Fab.
7	04523	R. Brown	Quartz	AJ #2	Opt. Fab.
8	04524	H. Lipson	NaCl	(1)	Opt. Fab.
9	04525	H. Lipson	MgF_2	OPTO#8	Opt. Fab.
10	04526	H. Lipson	NaCl	(4)	Opt. Fab.
11	04527	A. Armington	Quartz	SARP 2a,2b	Opt. Fab.
12	04528	C. Pitha	Plates	Agfa-Gevaert	
13	04529	H. Lipson	Quartz	D-14-45-1B	Opt. Fab.
14	04530	H. Lipson	Quartz	Russian	Opt. Fab.
15	04531	A. Armington	Quartz	AJ #2	Opt. Fab.
16	04532	J. Kennedy	InP	10:13-77 11:8-77 12:1-77	X-Ray:Fab.
17	04533	H. Lipson	MgF_2	OPTO#8	Opt. Fab.
18	04534	H. Lipson	MgF_2	OPTOVAC	Opt. Fab.
19	04535	J. Larkin	Al_2O_3	ManLabs Material	X-Ray:Fab
20	04536	H. Lipson	Quartz	A1-35 (2) each A2-33 A4-42 A12-35	X-Ray:Fab
21	04537	J. Kennedy	InP	10/13 11/8 12/1	Machine
22	04538	H. Lipson	Quartz	A-14-27 M_z A-14-27 M_{ii} Gr.III 5a	Opt. Fab.
23	04539	N. Pickering	Data		Data

Item	RADC No.	Requestor	Material	Specimen	Type of Service
24	04540	A. Golubovic	W Coils BC Crucible		Machine
25	04541	A. Golubovic	W Coils		Machine
26	04542	H. Posen		Spool Winders	Machine
27	04543	R. Hilton	InP	5:18	X-Ray:Fab
28	04544	B. Stiglitz	$LiNbO_3$	Mounted	Opt. Fab.
29	04545	J. Larkin	$Pb_2KNb_5O_{15}$	M. Brun PSU 3/78	X-Ray:Fab
30	03984	J. Bruce	$AlPO_4$	C-1	X-Ray:Fab
31	04546	C. Pitha	Brass/Glass	Absorption Cells	Machine
32	04547	R. Marshall	ZrO_2	(62.6 grams)	Analysis: X-Ray Diff.
33	04548	H. Lipson	ZrO_2	#4A	Opt. Fab.
34	04549	J. Adamski	Glass	##	Machine
35	04550	N. Pickering	Beam Blanking	Fixture	Machine
36	04551	H. Lipson	NaCl	##	Opt. Fab.
37	04552	F. Euler	Quartz	H-34	Opt. Fab.
38	04553	N. Pickering	YIG/GGG	#109	X-Ray:Fab.
39	04575	H. Lipson	NaCl	##	Opt. Fab.
40	04554	R. Marshall	Silicon	##	Opt. Fab.
41	04555	H. Lipson	Quartz	D14-45Da	Opt. Fab.
42	04556	N. Pickering	Fiber Optic Preforms		Analysis: Microprobe
43	04557	J. Comer	Quartz	Sawyer #1	Opt. Fab.
44	04558	H. Lipson	Quartz	D 14-45D	Opt. Fab.
45	04559	R. Hilton	InP	10:23:78	X-Ray:Fab.
46	04560	F. Euler	Quartz	H34-11	Opt. Fab.
47	04561	R. Hilton	InP	10:30:78	X-Ray:Fab.
48	04562	VOIDED			

Item	RADC No.	Requestor	Material	Specimen	Type of Service
49	04563	A. Armington	$AlPO_4$	B-2	X-Ray:Fab.
50	04564	N. Pickering	Glass	A9-14	Analysis: Emissions
51	04565	R. Marshall	ZrO_2	15-23	Analysis: Microprobe
52	04566	H. Lipson	Quartz	D14-45	Opt. Fab.
53	04567	H. Lipson	Quartz	D14-45	Opt. Fab.
54	04568	A. Armington	Quartz	AJ-delta 1	X-Ray:Fab.
55	04569	A. Armington	Quartz	Motorola 217-14	X-Ray:Fab.
56	04570	H. Posen	Fiber Optics Glass Preform		Opt. Fab.
57	04571	H. Lipson	MgF_2	1-5-6	Opt. Fab.
58	04572	N. Pickering	Glass Standards	A15-17	Analysis: Emission
59	04573	H. Posen	(Sb Compounds)		Thermodynamic Calc.
60	04574	A. Armington	$AlPO_4$	D-35	X-Ray:Fab.
61	04575	H. Lipson	NaCl	(2-35mm)	Opt. Fab.
62	04576	H. Lipson	Quartz	SARP D-14-45 (6)	Opt. Fab.
63	04577	H. Posen	Fiber Optics Preforms	RADC 9-12-32-34-42	Analysis: Microprobe
64	04578	H. Posen	Fiber Optics Preforms	RADC 9-12-32-34-42	Analysis: Microprobe
65	04579	R. Marshall	ZrO_2	Sample #1 and #2	Analysis: Emission
66	04580	R. Marshall	Pyrex Tube	Furnace Liners(54pcs)	Glass Fab.
67	04581	R. Brown	Quartz	AJΩ-2 (2)	Opt. Fab.
68	04582	N. Pickering		AMR-900 Beam Blanker	Machine
69	04583	A. Armington	Quartz	RD 21-48 (3)	X-Ray:Fab.

Item	RADC No.	Requestor	Material	Specimen	Type of Service
70	04584	N. Pickering		12 VU-Graphs	Art Work
71	04585	R. Hilton	InP	3:19:79 (16 seeds)	X-Ray:Fab.
72	04586	A. Golubovic	Pyrex Tube	Liners for Sputter System	Glass Fab.
73	04587	R. Marshall	Silicon	(2)-5 1/2 in. disks	Machine
74	04588	I. Bruce	Quartz	RD21-48 (3)	Opt. Fab.
75	04589	Marshall	ZrO_2	#13-#36-#38	Analysis: Emission
76	04590	Pitha	Film	AGFA 8E	
77	04591	Lipson	(4) Quartz	D-14-45 2aii (Li,Na,K doped)	Opt. Fab.
78	04592	Pickering	Machine Beam Blanker		Machine
79	04593	Friedman	(1) PtSi	LSD-29	Opt. Fab.
80	04594	Marshall	ZrO_2	I,II,III	Analysis: X-Ray Diff.
81	04595	Euler	Quartz	SARP K 14-45	X-Ray:Fab.
82	04596	Pickering	Prepare	VU-Graphs	Artwork
83	04597	O'Connor	Li_2GeO_2		Analysis: Microprobe
84	04598	Euler	Quartz	SARP PLf 1	X-Ray:Fab.
85	04599	Euler	(3) Quartz	SARP PLf 2	Opt. Fab.
86	04600	Euler	(2) Quartz	SARP II-BBA 18	Opt. Fab.
87	04601	Euler	(3) Quartz	SARP PLf 1	Opt. Fab.
88	04602	Friedman	(4) PtSi	LSD 19-29-49-62	Opt. Fab.
89	04603	Friedman	(1) PtSi	LSD-65	Opt. Fab.
90	04604	Pickering/ Yang	Optical Fiber	POL #2	Analysis: SEM/EDAX
91	04605	Comer	Special Consultation		Analysis: TEM

Item	RADC No.	Requestor	Material	Specimen	Type of Service
92	04606	Marshall	ZrO_2	ESM-CClpwd ESM-CCl xtal ESM-W1 xtal ESM-M1 xtal	Analysis: Emission
93	04607	Friedman	(1) PtSi	LSD-56	Opt. Fab.
94	04608	Armington	HgS	#2 (6.9 grams)	Analysis: X-Ray Diff.
95	04609	Armington	Quartz	RD-21 A/B/C	Analysis: Emission
96	04610	Marshall	ZrO_2	ESM-R1 xtal	Analysis: Emission
97	04611	Lipson	(6) Quartz	D 14-45 #43a Fast STD	Opt. Fab.
98	04612	Posen	Optical Fiber (3)	3360 #3#8#9	Analysis: SEM/EDAX
99	04613	Bruce	Quartz (3)	217-14-Q4/Q6	Opt. Fab.
100	04614	Brown	Li_2GeO_3	#04169	Opt. Fab.
101	04615	Posen	Optical Fiber (2)	3360 Run #2	Analysis: SEM/EDAX
102	04616	Brown	Quartz (1)	Swept Sample	Analysis: SEM/EDAX
103	04617	Drexhage	Glasses (1)	Zr/Ba/Th F	Analysis: SEM/EDAX
104	04618	Brown	Li_2GeO_3	#04169	Opt. Fab.
105	04619	Brown	Li_2GeO_3	#04169	X-Ray:Fab.
106	04620	Lipson	NaCl (6)	Dewar Windows	Opt. Fab.
107	04621	Lipson	$ZrO_2:Y_2O_3$	(11) Lots of Various Compositions	Opt. Fab.
108	04622	Drexhage	Glasses (4)	HBT:HZBT:HBL:ZBT	Opt. Fab.
109	04623	Marshall	Silicon (2)	#990378,#8969	Analysis: Vacuum Fusion
110	04624	Drexhage	Glasses (1)	HBT	Opt. Fab.
111	04625	Armington	Quartz (5)	Seed Plates	Opt. Fab.

Item	RADC No.	Requestor	Material	Specimen	Type of Service
112	04626	Quinlan	Feed Powders (6) ZrO_2:LaF_2:ThO_2	HfO_2:BaO:ThF_2	Analysis: Emission
113	04627	Drexhage	Glasses (2)	HBT:ZBT	Analysis: Emission
114	04628	Lipson	Aluminum (10)	Front Surface Mirror Blanks	Opt. Fab.
115	04629	Drexhage	Glass Powder	#25-#50	Analysis: Emission
116	04630	Hilton	InP Crystals	#6:19:78	X-Ray:Fab.
117	04631	Euler	Quartz	SARP H36-11	Opt. Fab.
118	04632	Marshall	ZrO_2	#46-#48	X-Ray:Fab.
119	04633	Drexhage	Glass Slug	HBT-012A	Opt. Fab.
120	04634	Drexhage	Glass Samples	HBT-009B ZBT-011A HZBT-013A	Analysis: Emission
121	04635	Marshall	ZrO_2	(doped 0.3% CeF_3)	Analysis: SEM/EDAX
122	04636	Fauth	Ge-Si Alloys	#168 #173 #175	Analysis: SEM/EDAX
123	04637	Hilton	InP Crystals	#12:5:79	X-Ray:Fab.
124	04638	Lipson	Quartz	E42-21	Opt. Fab.
125	04639	Lipson	ZrO_2(5 types)	+CeF +Nd_2O_3 +Er_2O_3 +Ho_2O_3 +V_2O_3	Opt. Fab.
126	04640	Armington	Quartz	X7-1/7-2/7-3/7-4	Opt. Fab. & Analysis: Emission
127	04641	Marshall	ZrO_2	+(Nd)	Opt. Fab.
128	04642	Drexhage	Fluoride Glasses	(5 lots)	Opt. Fab.
129	04643	Lipson	BaF_2	IR Window	Opt. Fab.
130	04644	Lipson	Quartz	Polished Specimen (1)	Opt. Fab.

Item	RADC No.	Requestor	Material	Specimen	Type of Service
131	04645	Marshall	Cubic ZrO_2	Polished Specimens (2)	Opt. Fab.
132	04646	Marshall	Cubic ZrO_2	Polished Specimens (2)	Opt. Fab.
133	04647	Lipson	Quartz	Polished Specimen(1)	Opt. Fab.
134	04648	Comer	Quartz	Electron Microscopy samples(6)	Opt. Fab.
135	04649	Comer	Quartz	as above (6)	Opt. Fab.
136	04650	Fauth	Ge/Si films	Depositions(7)	Analysis: SEM/EDAX
137	04651	Lipson	BaF_2	IR Windows (2)	Opt. Fab.
138	04652	Fauth	Ge/Si films	Depositions(2)	Analysis: SEM/EDAX
139	04653	Drexhage	Fluoride Glasses	(9 lots)	Opt. Fab.
140	04654	Drexhage	Fluoride Glasses	CU-1 (HBLF)	Analysis: Emission
141	04655	Marshall	Cubic ZrO_2	Sample #4	Analysis: Emission
142	04656	Brown	$Li_2 GeO_3$	Sample #04169 Q-Samples (3)	X-Ray: Fab.
143	04657	Lipson	Cubic ZrO_2	IR Samples (5)	Opt. Fab.
144	04658	Marshall	Fused Quartz	Pouring Ladle	Glass Working
145	04659	Marshall	Zr Metal (ManLabs supplied)	Pure metal chips	Analysis: EDAX
146	04660	Lipson	Cubic ZrO_2	IR sample (1)	Opt. Fab.
147	04661	Kahan	Quartz	Sample R-2	Opt. Fab.
148	04662	Kahan	Quartz	Q-samples(3) IR samples (3)	Opt. Fab.
149	04663	Golvbovic	LiF	UV sample (1)	Opt. Fab.
150	04664	Hilton	InP	#3:10:80 16 seed rods	X-Ray:Fab.
151	04665	Comer	Quartz	TEM samples(24)	Opt. Fab.
152	04666	Armington	Quartz	Seed Plates(6)	Opt. Fab.
153	04667	Lipson	Quartz	Polished Specimen(1)	Opt. Fab.

Item	RADC No.	Requestor	Material	Specimen	Type of Service
154	04668	Drexhage	Fluoride Glasses	(6 lots)	Opt. Fab.
155	04669	Lipson	Quartz	Polished Specimen(1)	Opt. Fab.
156	04670	Golubovic	Germanium	Sputter Target	Opt. Fab.
157	04671	Armington	Quartz	Boule X 5:Y-10 ESR samples(2) IR samples (6)	Opt. Fab.
158	04672	Marshall	Polycrystalline Silicon (ManLabs supplied)	2.8 Kgrams	Crystal Fab.
159	04673	Pickering	Cubic ZrO_2	Polished Specimen(1)	Opt. Fab.
160	04674	Golubovic	InP Wafers	#34-43-44	Analysis: Auger Profile
161	04675	Lipson	Quartz	(1) D 14-45 45a	Opt. Fab.
162	04676	Lipson	Quartz	(1) D14-45 Eb	Opt. Fab.
163	04677	Marshall	ZrO_2	(2) #62Nd #63Ce	Opt. Fab.
164	04678	Marshall	ZrO_2	(2) #83-86	Opt. Fab.
165	04679	Pitha	$Bi_{12}SiO_{20}$	(4)(100)(110) plates	X-Ray:Fab
166	04680	Fauth	Ge-Si Alloys	34 wafers	Analysis: SEM/EDAX
167	04681	Marshall	Si	Crucible	Machine
168	04682	Drexhage	Fluoride Glasses	(3) HBLPC	Opt. Fab.
169	04683	Drexhage	Fluoride Glasses	(4) Special Geometries: Index Ref. Wedges	Opt. Fab.
170	04684	Marshall	Alumina	Na doped Al_2O_3	Analysis: SEM/EDAX
171	04685	Armington	Quartz	QA4-P QA4-U (18) Geometries	Opt. Fab.
172	04686	Marshall	ZrO_2 Y_2O_3	(3) Stock Powder	Analysis: Emission

Item	RADC No.	Requestor	Material	Specimen	Type of Service
173	04687	Marshall	ZrO_2	#85-#86	Analysis: X-Ray Diff.
174	04688	Lipson	NaCl	(2) Windows	Opt. Fab.
175	04689	Lipson	Quartz	(6) D14-45 39b Boule X-11	Opt. Fab.
176	04690	Hilton	InP	#6:2:80 (Seed rods)	X-Ray:Fab
177	04691	Lipson	Quartz	(2) D14-45 #39 a iii	Opt. Fab.
178	04692	Armington	Quartz	(7) F2-1	Opt. Fab.
179	04693	Lipson	Quartz	(3) "Amethyst"	Opt. Fab.
180	04694	Sahagian	Cs_2NaYCl_6	(4)Water Soluble Salts	Opt. Fab.
181	04695	Marshall	ZrO_2	(5) #16,17,18, 20,34C	Analysis: X-Ray Fluorescence
182	04696	Drexhage	Fluoride Glasses	(13) samples	Opt. Fab.
183	04697	Lipson	Quartz	(1) F42-21	Opt. Fab.
184	04698	Euler	Quartz	SICN 203	Opt. Fab.
185	04699	Drexhage	Glasses	HBZLR(6)	Opt. Fab.
186	04700	Marshall	GaAs	#53 (Seeds)	X-Ray:Fab.
187	04701	Marshall	ZrO_2	Ho doped	Opt. Fab.
188	04702	Marshall	Silicon	DC poly	Machine
189	04703	Armington	Quartz	Q A5b	Opt. Fab.
190	04704	Marshall	Ge/Si	Cruc. Alloy	Analysis: SEM/EDAX
191	04705	Marshall	ZrO_2	18 lots	Opt. Fab.
192	04706	Lipson	ZrO_2	#1	Analysis: SEM/EDAX
193	04707	Marshall	ZrO_2	26 lots	Analysis: SEM/EDAX
194	04708	Fitzgerald	Pt-Si	10 diffusion couples	Analysis: Auger Profile

Item	RADC No.	Requestor	Material	Specimen	Type of Service
195	04709	Pickering	ZrO_2	Ce doped	Opt. Fab.
196	04710	Euler	Quartz	D14-45 Dh	X-Ray:Fab.
197	04711	Euler	Quartz	QNU-1	X-Ray:Fab.
198	04712	Drexhage	Glasses	ZHBLF (14)	Opt. Fab.
199	04713	Drexhage	Glasses	HBL (4)	Opt. Fab.
200	04714	Lipson	Quartz	D 14-45 Dh(3)	Opt. Fab.
201	04715	Lipson	Resonators Quartz	FSC/Bliley	Machine

VI. APPENDIX

CALCULATION OF THE VAPOR-LIQUID-ZINCBLENDE EQUILIBRIA IN THE CADMIUM-TELLURIUM-MERCURY SYSTEM*

CALCULATION OF THE VAPOR-LIQUID-ZINCBLENDE EQUILIBRIA IN THE CADMIUM-TELLURIUM-MERCURY SYSTEM*

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1. Introduction

The II-VI compounds of $Cd_{0.5}Te_{0.5}$ and $Hg_{0.5}Te_{0.5}$ form a series of cubic zincblende solid solutions which offer the attractive property of a variable band gap depending upon composition. The $(Cd,Hg)_{0.5}Te_{0.5}$ solid solution displays band gaps which run in a nearly linear fashion between the wide gap semiconductor $Cd_{0.5}Te_{0.5}$ (Eg=1.6 eV) and the semi metallic compound $Hg_{0.5}Te_{0.5}$ which can be considered to be a semiconductor with a negative band gap (1). Alloys of $Cd_{0.1}Hg_{0.4}Te_{0.5}$ and $Cd_{0.2}Hg_{0.3}Te_{0.5}$ exhibit band gaps ranging from 0.1 to 0.5 eV respectively and are of particular interest for detection of infrared radiation in the 2 to 20 micron range. The growth of such alloy compositions from the melt presents some difficulties due to the "width" of the two phase liquid plus solid field along the $Cd_{0.5}Te_{0.5}$-$Hg_{0.5}Te_{0.5}$ quasi binary join. Liquid phase epitaxial (LPE) growth methods have been employed to circumvent this problem(1) but controlled growth requires a knowledge of the tie-lines between the alloy compound and the liquid. Such information can be generated experimentally, but with considerable effort. Alternatively, it is possible to apply the CALPHAD method (2) which has been applied to a very wide range of systems, for calculating the ternary Cd-Te-Hg system from a knowledge of the component binary systems in

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* This work was carried out under Contract F 19628-78-C-0060 with the Electronic Systems Division, RADC-AFSC-Hanscom Field, Bedford, Mass. 01730

order to provide the required information on tie-line composition. The description provided below provides an account of such calculations.

2. Description of the Vapor, Liquid and Zincblend Phases

Table 1 summarizes the current descriptions of the liquid(L), vapor(V) and zincblende(S), phases in the cadmium-tellurium-mercury system as a function of temperature (T°K), pressure (P atmospheres), atomic fraction tellurium(x), and atomic fraction of mercury (y). These equations, along with the associated lattice stability values relating the free energy of the vapor, liquid, fcc and stable forms of cadmium, tellurium and mercury have been assembled by employing existing (3-7) thermochemical and phase diagram data for the pure elements and binary systems. Figures 1-6 show the partial binary phase diagrams computed for the Te-Cd, Hg-Cd and Te-Hg systems at P=1 atmosphere and P=16 atmospheres. These phase diagrams follow directly from the ternary equations listed in Table 1 when they are reduced to binary systems for each of the edge binary systems in question. The small ternary terms assigned to the liquid phase (-33472xy(1-x-y)) and the zincblende phase (-4180y (1-2y)) Joules/g.at. were chosen in conformity with the experimental results along the $Cd_{0.5}Te_{0.5}$-$Hg_{0.5}Te_{0.5}$ quasi-binary join shown in Figures 7 and 8. Since the maximum value of these terms is attained at x=0.5 and y=0.25 it is apparent that the ternary correction term is at most about ≈1000 Joules/g.at. for the liquid phase and -300 Joules/g.at. for the zincblende phase at the x=0.5, y=0.25 composition.

Figures 9-11 display calculated isothermal sections in the Cd-Te-Hg systems between 1 and 74 atmospheres and at temperatures ranging from 773°K to 1213°K. These calculated isothermal sections display the tie-lines between the zincblende and liquid phases in addition to the three phase vapor-liquid-zincblende fields which are especially important in crystal

TABLE I

SUMMARY OF FREE ENERGY EQUATIONS DESCRIBING THE VAPOR LIQUID AND ZINC BLENDE PHASES IN THE CADMIUM-TELLURIUM-MERCURY SYSTEM
(All units in joules per gram atom (mole of atoms), °K)

L=Liquid Phase, V=Vapor Phase, S=Zincblende Phase, A=fcc
R=Rhombohedral (Stable Hg), T=Trigonal (Stable Te), E=hcp (Stable Cd)
x=atom fraction Te, y=atom fraction Hg, P=Pressure (Atmospheres)
R=8.315 J/g.at°K

Lattice Stability Values

$G^L_{Hg} - G^R_{Hg} = 2292-9.832T$; $\bar{T}=234K$

$G^A_{Hg} - G^R_{Hg} = 2297-1.454T$

$G^V_{Hg} - G^L_{Hg} = 59174-93.303T+RT\ell nP$

$G^L_{Te} - G^T_{Te} = 17489-24.184T$; $\bar{T}=723K$

$G^A_{Te} - G^T_{Te} = 17489-15.816T$

$\frac{1}{2}G^V_{Te_2} - G^L_{Te} = 58409-45.982T+0.5RT\ell nP$

$G^L_{Cd} - G^E_{Cd} = 6192-10.418T$; $\bar{T}=594K$

$G^A_{Cd} - G^E_{Cd} = 1924-2.050T$

$G^V_{Cd} - G^L_{Cd} = 102,520-98.659T+RT\ell nP$

Ternary Phases

$$G^L = (1-x-y)G^L_{Cd} + xG^L_{Te} + yG^L_{Hg} + RT\,[(1-x-y)\ell n(1-x-y)+x\ell nx+y\ell ny]$$
$$+ x(1-x-y)(1-y)^{-1}\,[(30962+5.02T)x+(3514+16.74T)y]+x(-75312-20.92T)]$$
$$- xy(x+y)^{-1}\,[35982x+(3514+16.74T)y] + y(1-x-y)\,[-10878+4.184T] - 33472\,xy(1-x-y)$$

$$G^V = (1-x-y)G^V_{Cd} + 0.5x\,G^V_{Te_2} + y\,G^V_{Hg}$$
$$+ RT((1-x-y)\ell n(1-x-y)+x\ell nx+y\ell ny)$$

$$G^S = (0.5-y)\,G^A_{Cd} + 0.5\,G^A_{Te} + y\,G^A_{Hg} + (1-2y)\,[-61191+13.075T]+2y\,-26798+7.11T]$$
$$+ RT[y\ell ny + (0.5-y)\ell n(0.5-y)-0.5\ell n0.5] - 4180y(1-2y)$$
$$0 \leq y \leq 0.5$$

TABLE 2

COMPARISON OF CALCULATED AND OBSERVED (6) FREE ENERGY OF FORMATION AT 298F

Compound	ΔH [298]	ΔS [298]
$Cd_{0.5}Te_{0.5}$	-50800 ± 1300 (obs) -51500	-4.18 ± 1.25 (obs) -4.14
$Hg_{0.5}Te_{0.5}$	-15900 ± 2100 (obs) -18050	-6.28 ± 1.26 (obs) -3.39

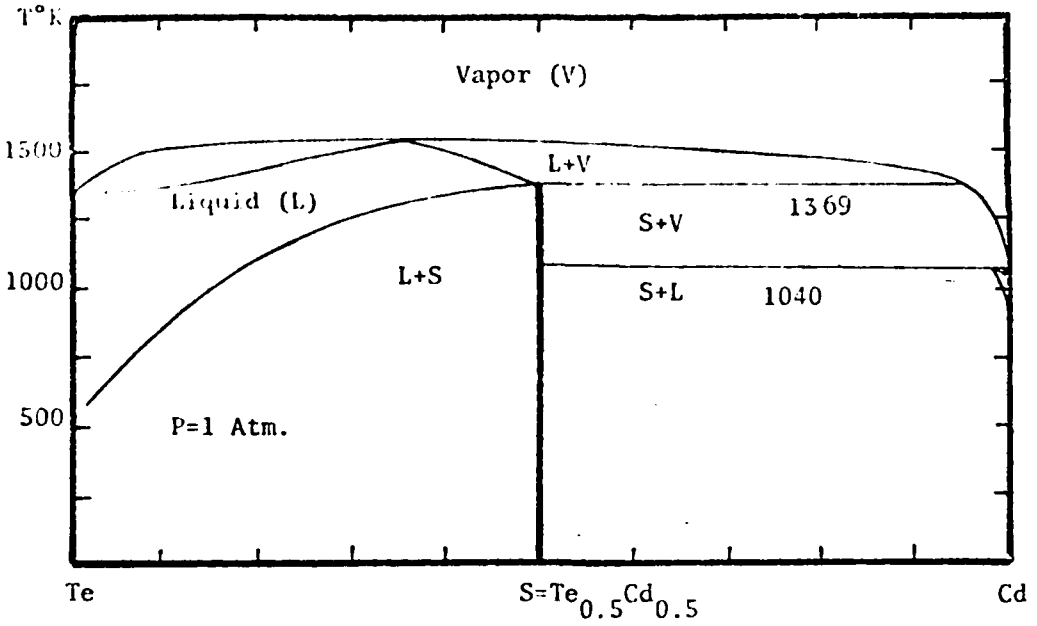


Figure 1 Calculated Partial Te-Cd Phase Diagram at 1 Atmosphere

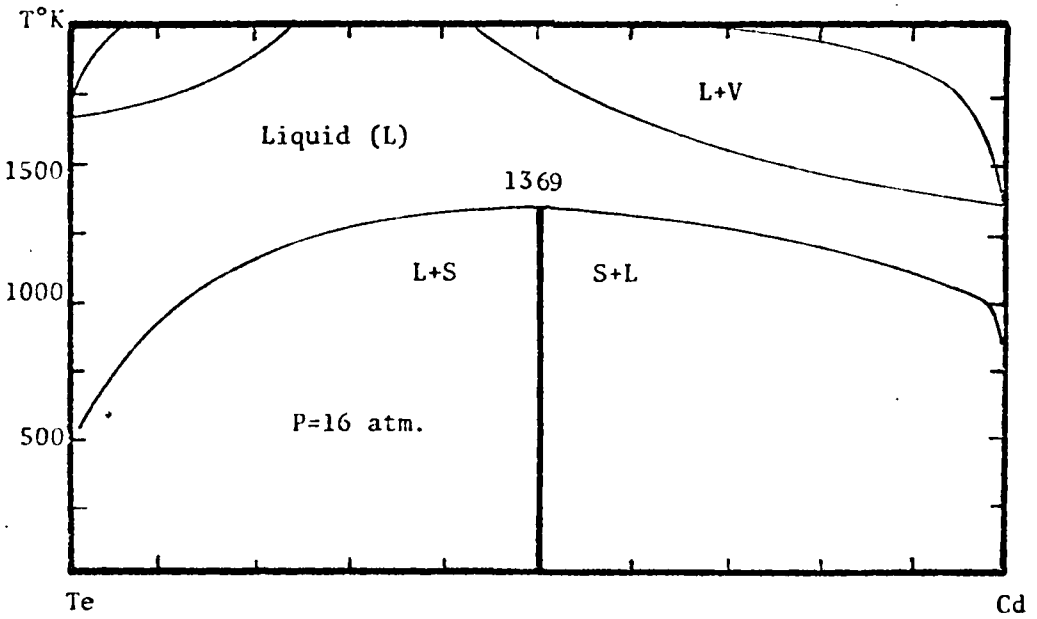


Figure 2 Calculated Partial Te-Cd Phase Diagram at 16 Atmospheres.

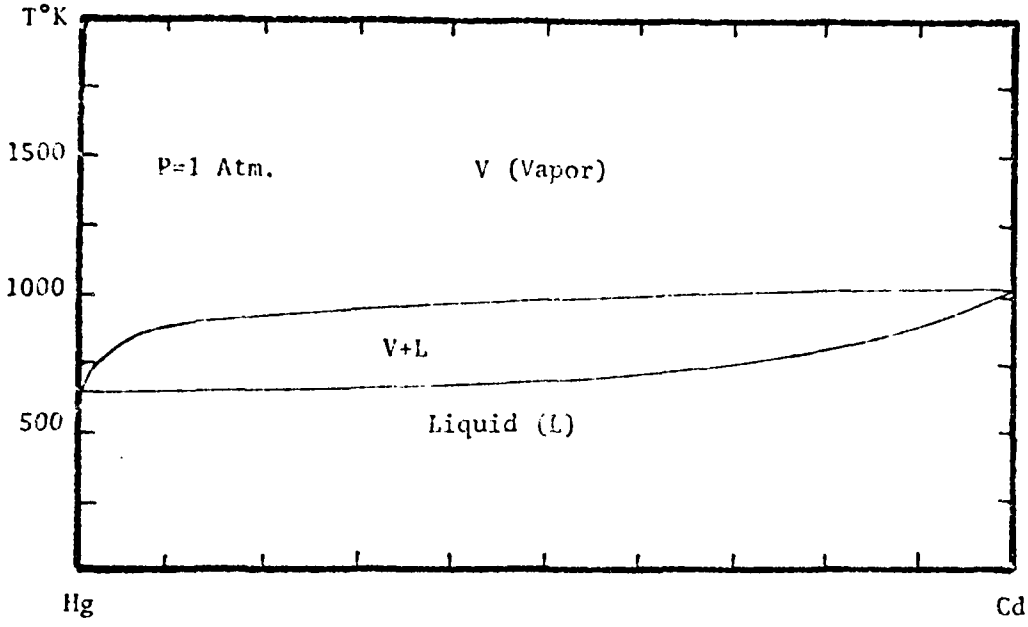


Figure 3 Calculated Partial Hg-Cd Phase Diagram at 1 Atmosphere

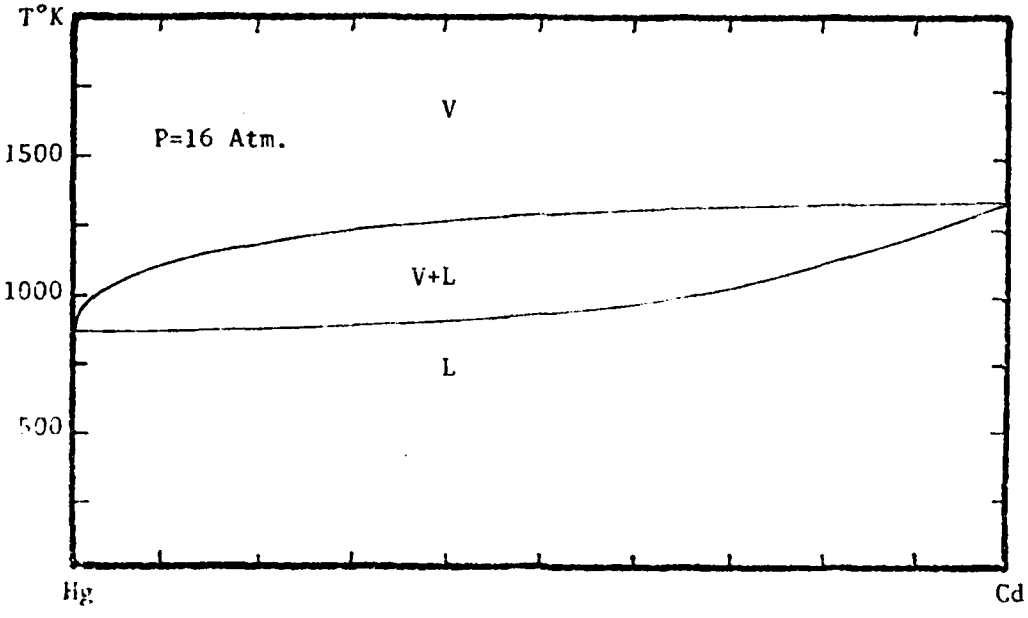


Figure 4. Calculated Partial Hg-Cd Phase Diagram at 1 Atmosphere

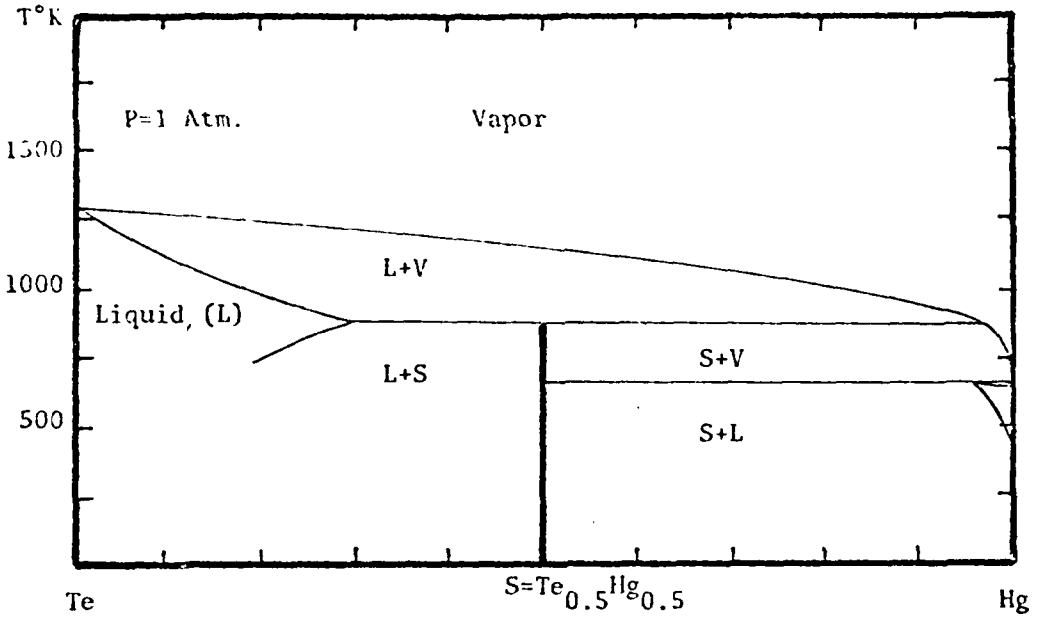


Figure 5 Calculated Partial Te-Hg Phase Diagram at 1 Atmosphere

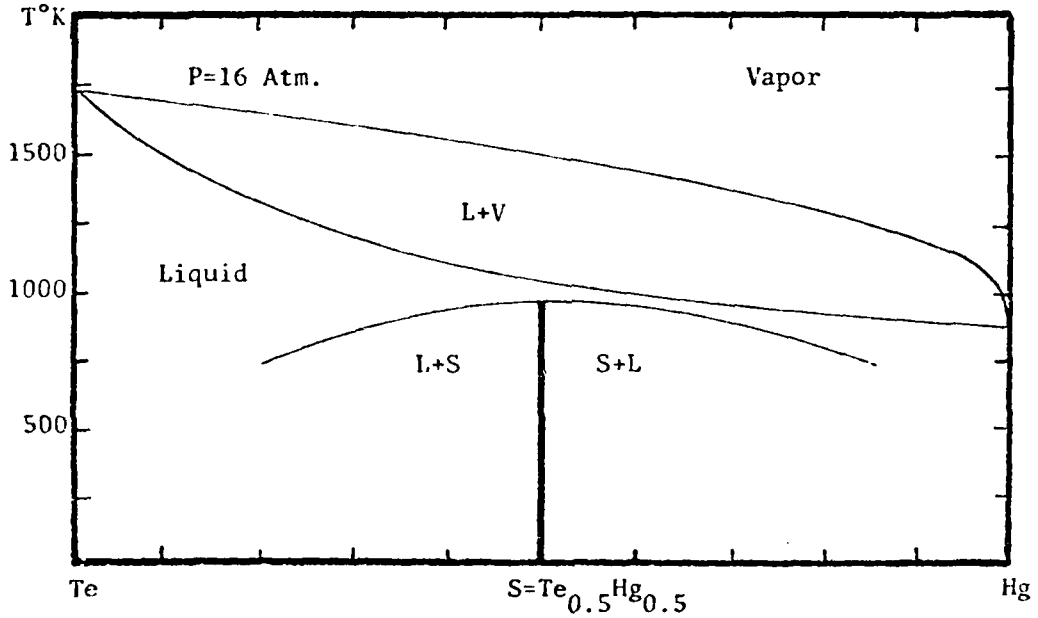
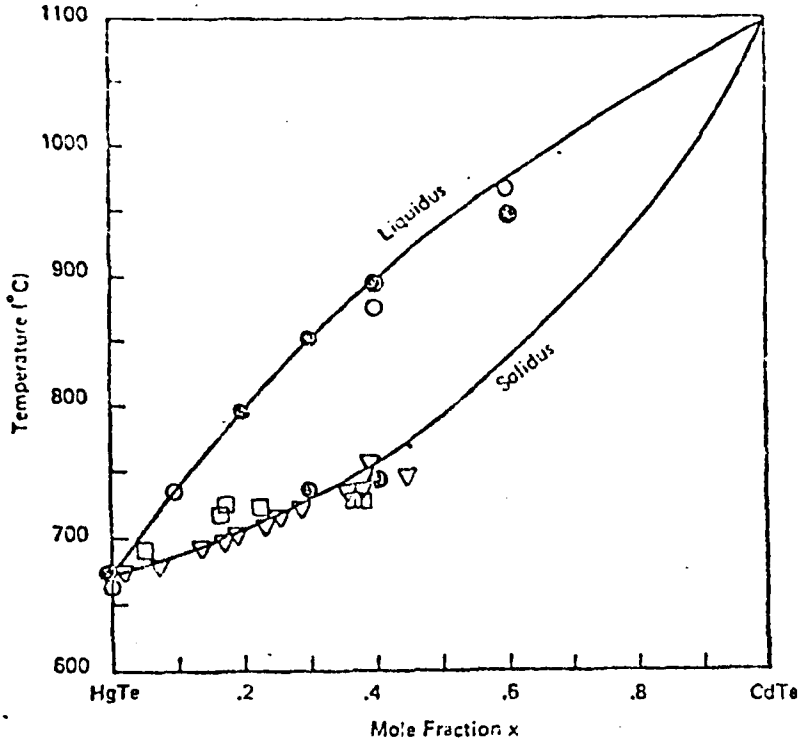


Figure 6 Calculated Partial Te-Hg Phase Diagram at 16 Atmospheres.



● This Investigation – Steininger(8)
○ Liquidus Data – Blair and Newnham (9)
▽ Solidus Data – Harman and Strauss (10)
□ Solidus Data – Schmit and Speerschneider (11)

Figure 7. Liquidus and Solidus Curves for Pseudo-binary $Hg_{1-x}Cd_xTe$ Compositions. (8)

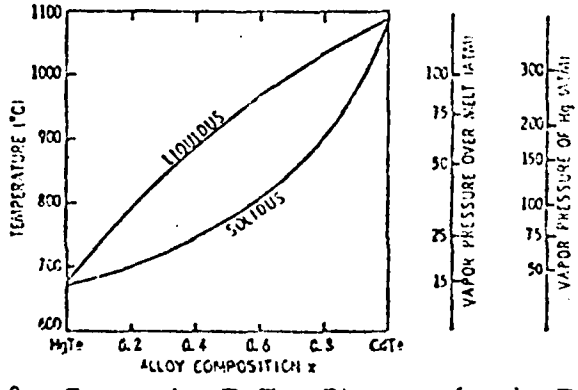


Figure 8. Composite P-T-x Diagram for the Pseudo-binary HgTe-CdTe System. (8)

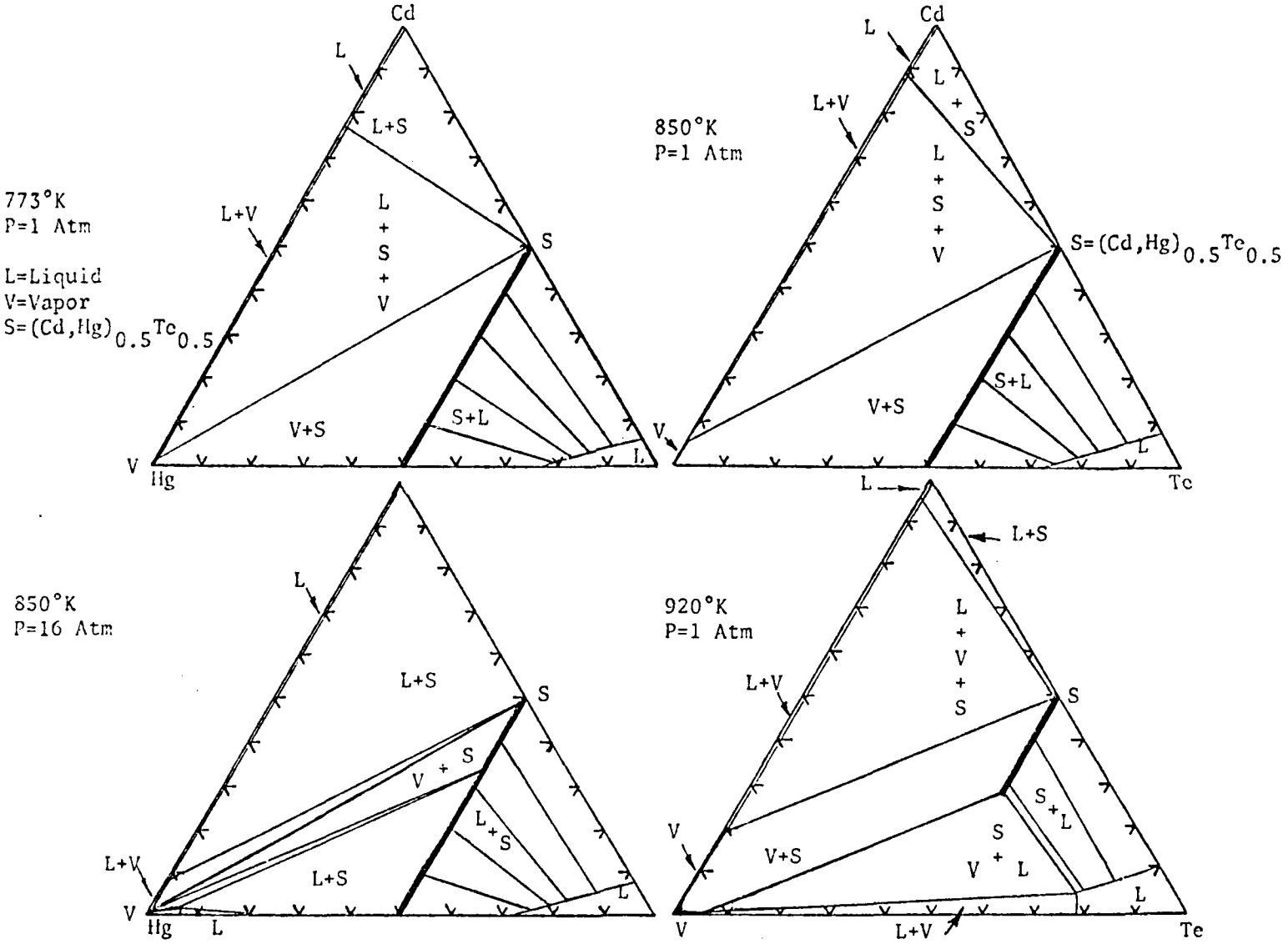


Figure 9 Calculated Isothermal Sections in the Cd-Te-Hg System

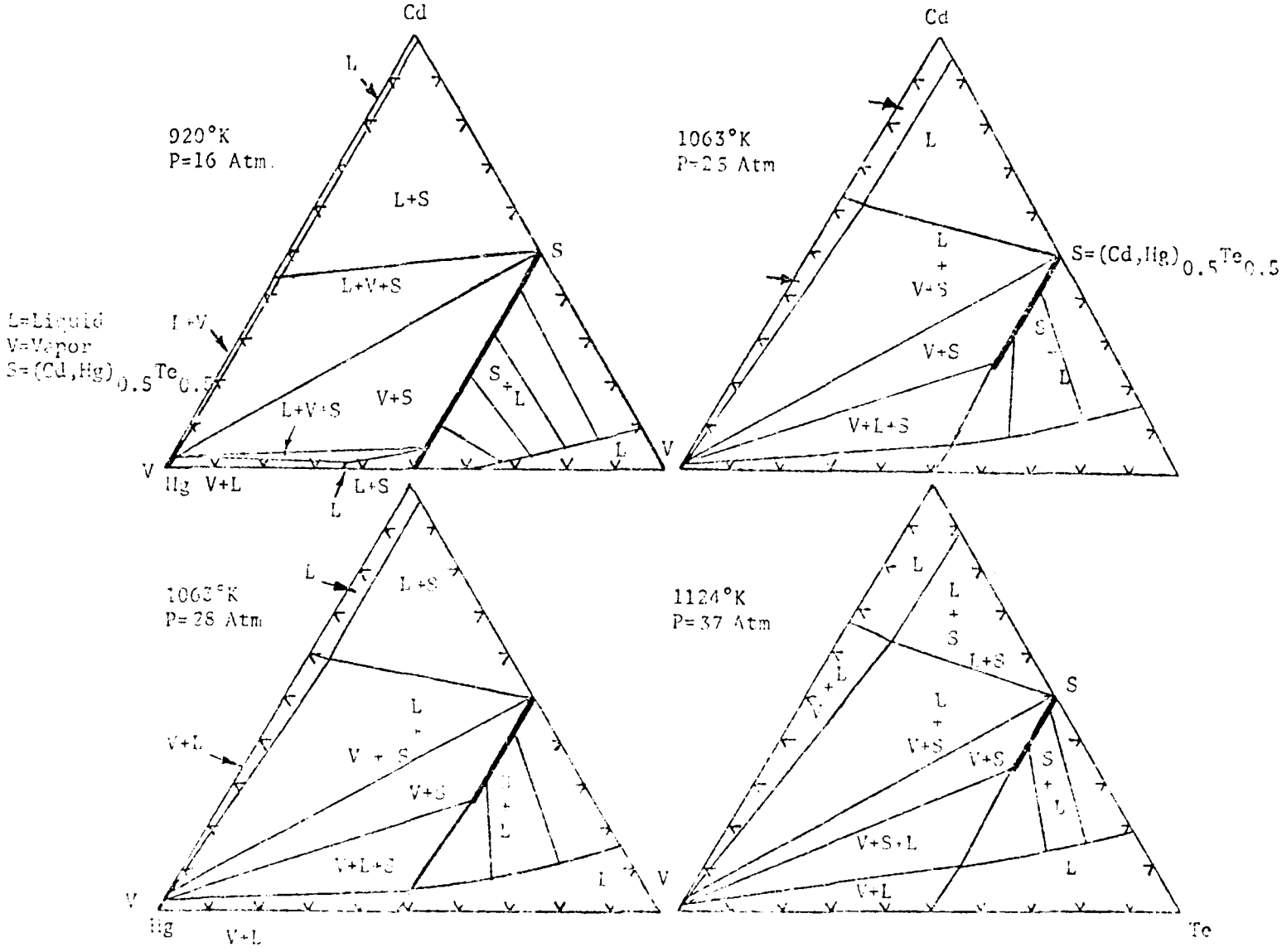


Figure 10 Calculated Isothermal Sections in the Cd-Te-Hg System

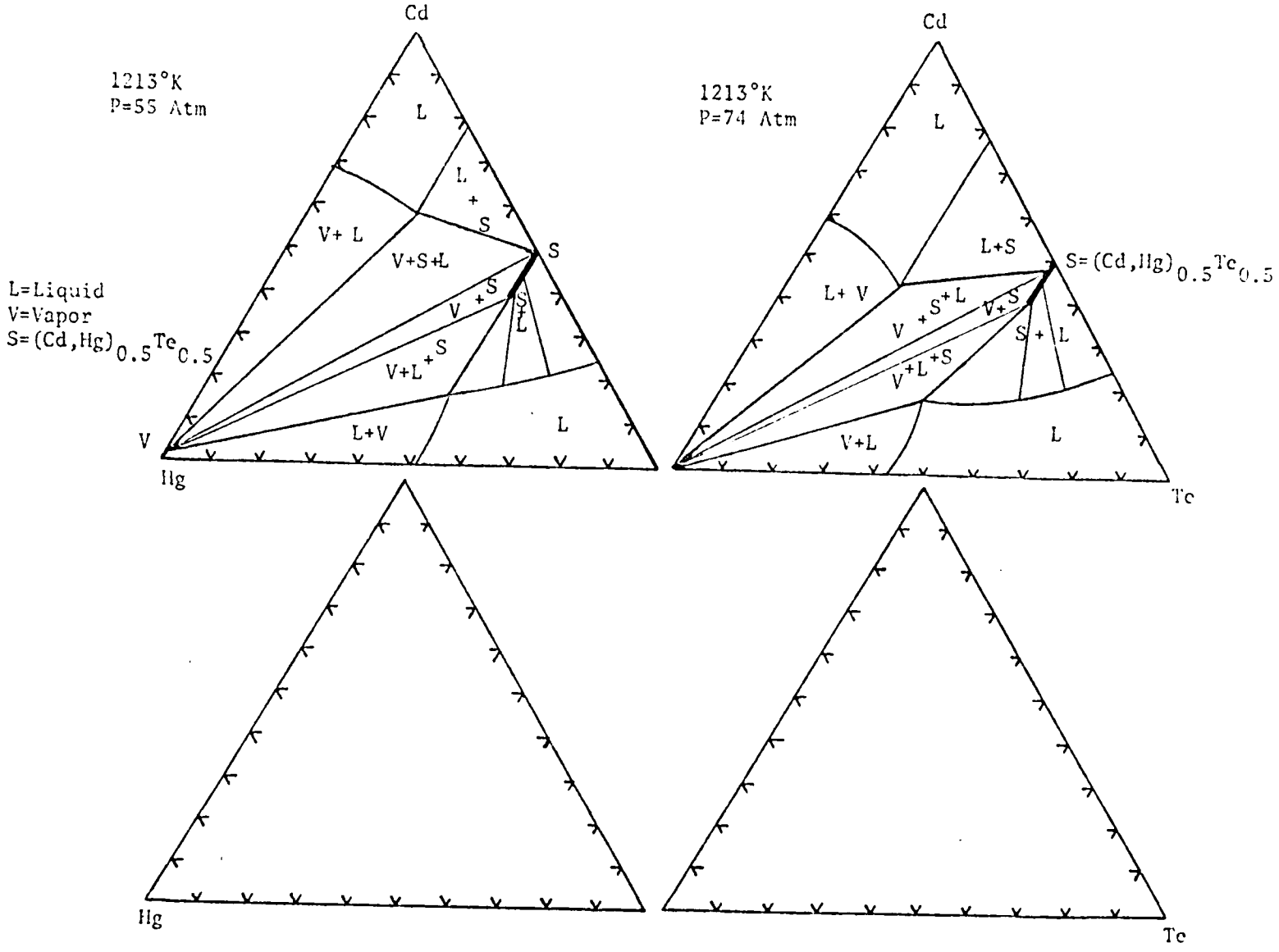


Figure 11 Calculated Isothermal Sections in the Cd-Te-Hg System

growth operations. The calculations of tie lines can be compared directly with the recent experimental results of Mroczkowski and Vydyanath who determined tie line compositions by means of "closed tube tipping experiments". In these experiments crystals of the zincblende phase of fixed composition are equilibrated with liquid phase in a graphite boat. After equilibration the temperature was reduced 5°C to 7°C, and the liquid decanted. Subsequent electron microprobe analysis of the concentration profiles along the length of the crystal (from the zincblende single crystal phase into the polycrystalline phase which forms when the contact liquid freezes) permits determination of the tie line compositions (1). At 818°K the following comparison can be made between the calculated and observed tie lines.

	Zincblende		Liquid	
Atomic Percent	Hg	Cd	Hg	Cd
Observed (1)	32.5	17.5	20.3	2.3
Calculated	32.5	17.5	18.0	3.4
	37.5	12.5	20.7	2.5

This excellent comparison provides an independent check of the description of the liquid and zincblende free energies shown in Table 1. These equations can be used to compute the liquid-vapor-zincblende equilibria over a wide range of temperature and pressure which can be used to define the conditions for stable conventional and LPE growth of Te rich and Te poor $(Cd,Hg)_{0.5}Te_{0.5}$ compositions.

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United States Air Force
Hanscom AFB, Mass. 01731